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Differential cross sections for $\bar{e}$ - CO elastic scatttering

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Abstract : In a recent investigation, Raj and Kumar [*Phys. Lett.* **A282**, 284 (2001)] modified the absorption potential of Staszewska *et al* [*Phys Rev* **A28** 2740 (1983)] in such a way that it yielded the best agreement between theory and experiment for elastic cross sections when applied to $\bar{e}$ - O_2 scattering over a wide incident energy range In the present investigation, the same modified absorption potential of Raj and Kumar has been employed to obtain the elastic differential cross sections (EDCS) for electron scattering by CO molecules at intermediate energies (100-800 eV). The independent atom model alongwith partial waves has been used for these calculations The present results of EDCS are in fairly good agreement with the experimental data.

Keywords : Differential cross section, electron, CO molecule, independent atom model

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In recent past, a number of investigations for $\bar{e}$-atom/ molecule elastic scattering have been carried out [1-5] which included absorption effects through the absorption potential of Staszewska *et al* [2]. All these investigations confirm that this absorption potential is too attractive and hence overestimate the flux loss to the electronic excited states for large angle scattering, particularly at high incident energies. Consequently, it under estimated the experimental values of elastic differential cross sections. Furthermore, the effect of absorption potential was found to increase instead of decreasing with increasing incident energy [Figures 1 (a)-1(d)] of Ref. [1]. Hence, to improve agreement between theory and experiment, contribution of the absorption potential of Staszewska et al to DCS should be reduced. Keeping these points in mind, Raj and Kumar [1] modified this absorption potential and obtained best agreement between theory and experiment for $\bar{e}$-O_2 elastic scattering. Hence, it will be worthwhile to test the applicability of this modified absorption potential for $\bar{e}$-CO elastic scattering.

For the present calculations, independent atom model has been employed. In this model, EDCS averaged over all orientations of inter nuclear axis for $\bar{e}$-CO scattering is given by [6]:

$$I_{ind}(\theta) = I_C(\theta) + I_O(\theta) + \left(f_C^*(\theta) f_O(\theta) + f_c(\theta) f_O^*(\theta)\right) \times \sin Kr_e / Kr_e \ldots, \quad (1)$$

where the suffixes C and O stand for carbon and oxygen atoms, respectively. $f(\theta)$ and $I(\theta)$ are the atomic scattering amplitude and differential cross section, respectively. $K(= 2\,k \sin\theta/2)$ is the magnitude of the change in momentum vector of the incident electron due to scattering. r_e is the equilibrium internuclear distance between C and O atoms. Eq. (1) assumes that each atom of the molecule scatters as if it were free and multiple scattering is negligible. In the present investigation, partial wave method has been employed to obtain $f(\theta)$ for constituent atoms of molecule, as given by [4,6].

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{N}(2l+1)\left(e^{i\eta_l}\sin\eta_l - \eta_l^B\right)P_l(\cos\theta) + f_{dp}^B(\theta), \quad (2)$$

where η_l^B and $f_{dp}^B(\theta)$ are the first Born phase shifts and scattering amplitude, respectively, due to long range dynamic polarization potential. $P_l(\cos\theta)$ are Legendre polynomial and N is an integer such that $\eta_l \sim \eta_l^B \leq 2\%$. If this condition is not satisfied at any incident energy, maximum value of N is taken to be 30. Above expression takes contribution of first few partial waves say $(N+1)$ exactly and includes the contribution of the

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remaining ones through first Born approximation.

To obtain phase shifts η_l for l^{th} partial wave, the following differential equation is numerically solved under proper boundary conditions:

$$\frac{d^2}{dr^2} + k^2 - V_{opt}(r) - \frac{l(l+1)}{r^2} \Big] . f_l(r) = 0, \qquad (3)$$

where k^2 is the energy of the incident electron (atomic units have been used where length is expressed in a_0 and energy in Rydbergs). The optical potential $V_{opt}(r)$ replaces the constituent atom and is supposed to mock all the types of electron- atom interactions. In general, it is complex energy-dependent and non-local. However, in the present work, it is taken as a spherically symmetric, local, complex and energy-dependent, given by :

$$V_{opt}(r) = V_{st}(r) + V_{ex}(r) + V_{dp}(r) + iV_{abs}^{m}(r), \qquad (4)$$

where V_{st}, V_{ex}, V_{dp} and V_{abs}^{m} are the static, exhange, dynamic polarization and modified absorption potential, respectively. The details of these potentials may be found elsewhere [1,4,5]. After obtaining $f(\theta)$ for C and O atoms, $I_{CO}(\theta)$ was calculated from eq. (1).The present results of EDCS alongwith available experimental data [7-10] and other theoretical results of Kamna Yadav [11], are displayed in Figures. 1-3 for incident energies ranging from 100-800 eV.

In Figure 1, present results of EDCS obtained with modified absorption potential (full curve) at incident energies 100, 200

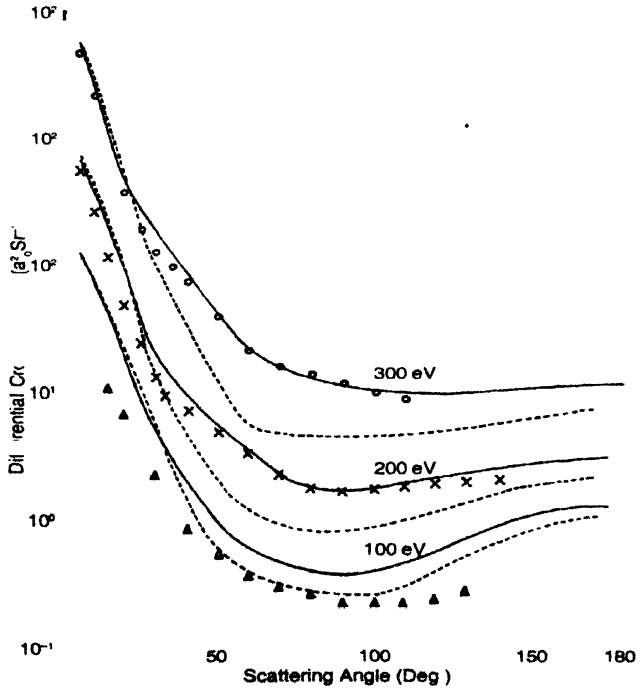

Figure 1

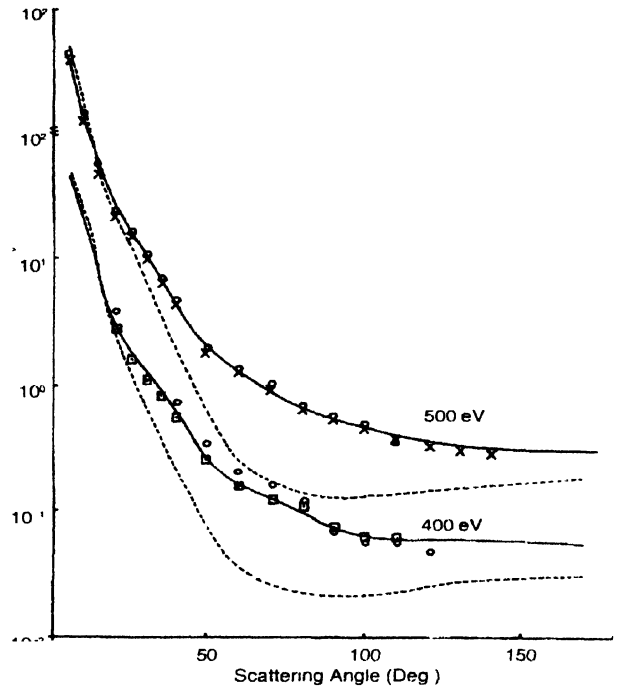

Figure 2

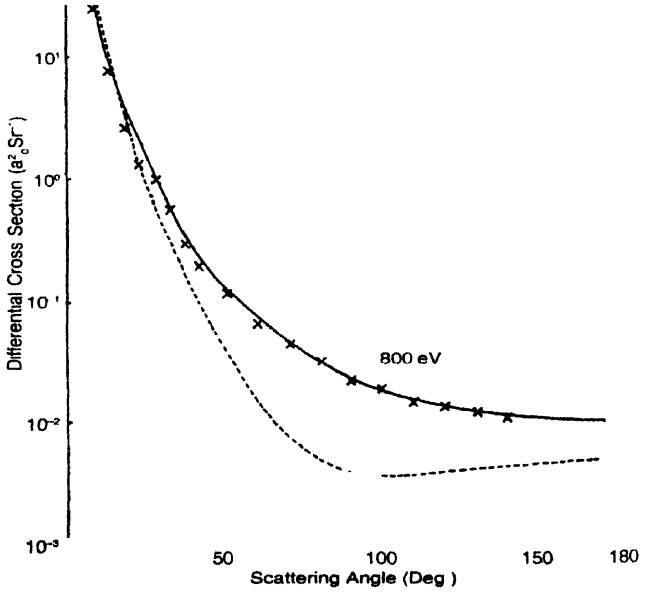

Figure 3

Figures 1-3 : Differential cross sections for $\bar{e}$ - CO elastic scattering at various incident energies.
Theoretical: – Present results with modified absorption potential. .....Results of Kamna Yadav [11] with absorption potential of Staszewska *et al* [2].
Exp. Data: □ Arnot [7], O Bromberg [8], X DuBois and Rudd [9], Δ Tanaka *et al* [10]

and 300 eV have been plotted. The experimental data of Tanaka *et al* [10]at 100 ev (Δ), DuBois and Rudd [9] at 200 eV (X) and of Bromberg [8] at 300 eV (O), are also plotted. The theoretical results of Kamna Yadav [11] (broken curve), obtained with absorption potential of Staszewska *et al* [2], are also included for comparison. It is evident from Figure 1 that at 100 eV, the theoretical values of EDCS of Kamna Yadav [11] are in good agreement with the experimental data of Tanaka *et al* [10]. Our values are slightly higher than the experimental data [10]. At 200 eV, the present values of EDCS are in good agreement with the experimental data of DuBois and Rudd [9]. The theoretical values of Kamna Yadav [11] are much smaller than the experimental data in the middle angular region. Similarly, the data of Bromberg [8] at 300 eV is in very good agreement with the present values of EDCS where as the values of Kamna Yadav are again much smaller than the experimental data. It is evident from Figures 2 and 3 also that the present theoretical values of EDCS are in excellent agreement with the data of Bromberg [8] at 400 eV and with the data of DuBois and Rudd [9] at 500 and 800 eV. It may be noted that as the incident energy increases, the difference between the theoretical values of Kamna Yadav and the experimental data increases. On the other hand, the present values of EDCS obtained with modified absorption potential show increasingly better agreement with all the data and at all incident energies.

Thus, it is concluded that the use of modified absorption potential in the present investigation has yielded a better agreement with the experimental data at all incident energies investigated except at 100 eV. The applicability of the modified absorption potential to other targets is under investigation.

Acknowledgment

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